Butanamide, 4-hydroxy-

927-60-6 | DTXSID5061297

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.08 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.95e-01

Confidence level: 8.30e-01

Nearest Neighbors from the Training Set

Image not found
4-Aminobutanoic acid
Measured: 12.6
Predicted: 9.58

Image not found
beta-Aminobutyric acid
Measured: 9.70
Predicted: 9.12

Image not found
beta-Alanine
Measured: 6.12
Predicted: 7.73

Image not found
5-Aminovaleric acid
Measured: 8.54
Predicted: 8.01

Image not found
Diethylene glycol
Measured: 9.42
Predicted: 8.06